



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:41 AM UTC

PDB ID : 4E1L / pdb\_00004e1l  
Title : Crystal structure of Acetoacetyl-CoA thiolase (thlA2) from *Clostridium difficile*  
Authors : Anderson, S.M.; Wawrzak, Z.; Kudritska, M.; Peterson, S.N.; Anderson, W.F.; Savchenko, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2012-03-06  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

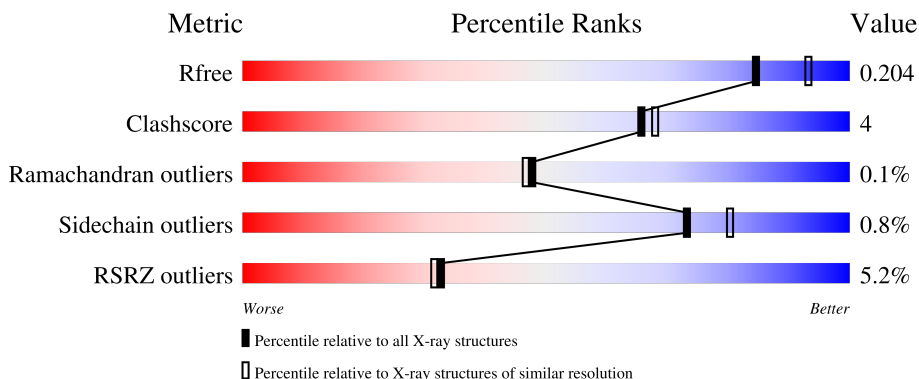
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

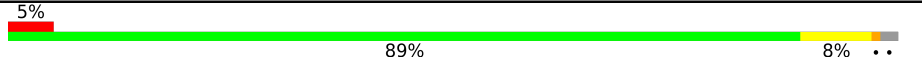
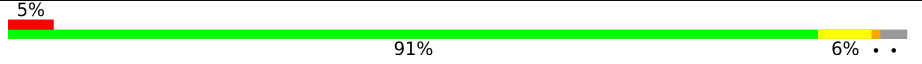


The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	395	 5% 89% 8% ..
1	B	395	 5% 91% 6% ..
1	C	395	 5% 83% 8% • 8%
1	D	395	 6% 83% 9% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	D	408[B]	-	-	X	-
2	IOD	D	409	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11993 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetoacetyl-CoA thiolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	2878	1804	499	561	14	0	3	0
1	B	384	2831	1775	492	550	14	0	1	0
1	C	363	2668	1674	458	524	12	0	1	0
1	D	364	2678	1676	467	523	12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q183B0
A	-1	ASN	-	expression tag	UNP Q183B0
A	0	ALA	-	expression tag	UNP Q183B0
B	-2	SER	-	expression tag	UNP Q183B0
B	-1	ASN	-	expression tag	UNP Q183B0
B	0	ALA	-	expression tag	UNP Q183B0
C	-2	SER	-	expression tag	UNP Q183B0
C	-1	ASN	-	expression tag	UNP Q183B0
C	0	ALA	-	expression tag	UNP Q183B0
D	-2	SER	-	expression tag	UNP Q183B0
D	-1	ASN	-	expression tag	UNP Q183B0
D	0	ALA	-	expression tag	UNP Q183B0

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	I	0	2
			17	17		
2	B	14	Total	I	0	1
			15	15		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	15	Total I 15 15	0	0
2	D	14	Total I 17 17	0	2

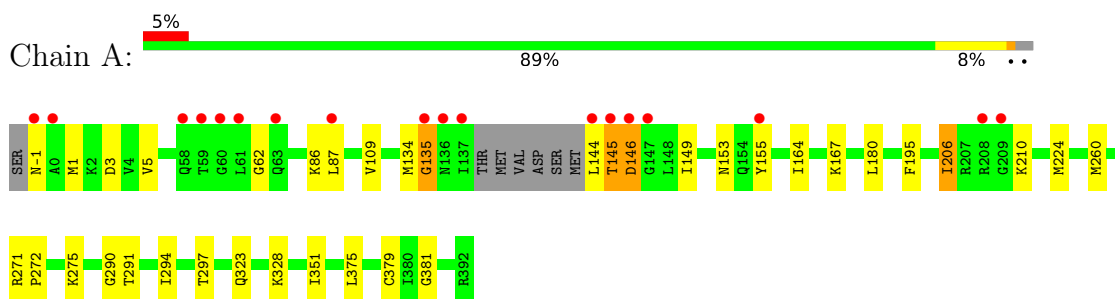
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	242	Total O 245 245	0	3
3	B	259	Total O 259 259	0	0
3	C	243	Total O 243 243	0	0
3	D	127	Total O 127 127	0	0

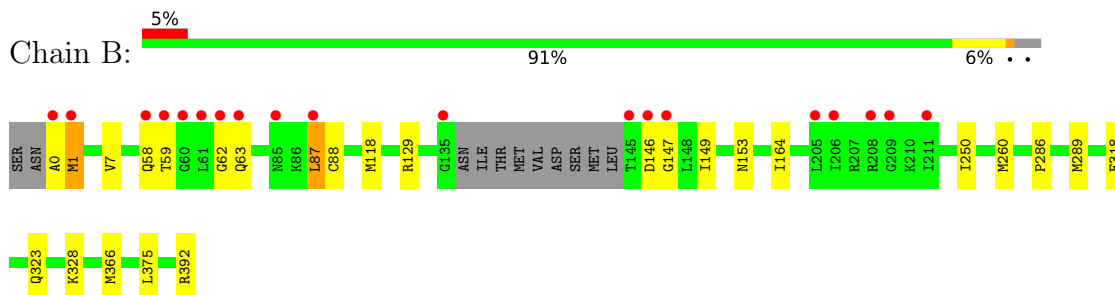
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

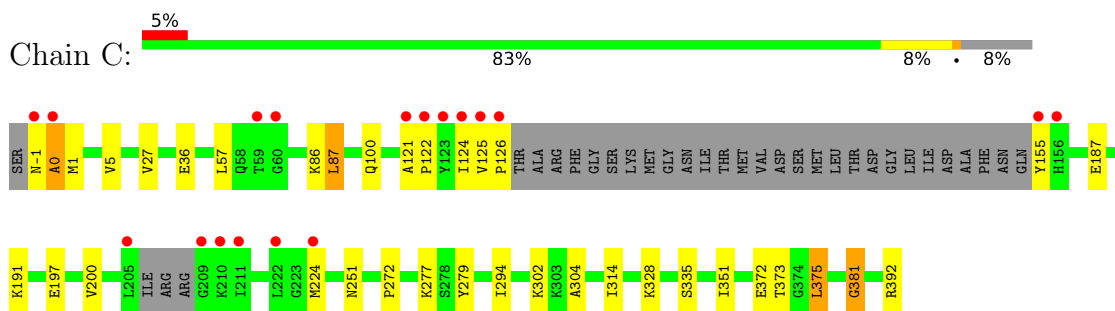
- Molecule 1: Acetoacetyl-CoA thiolase 2



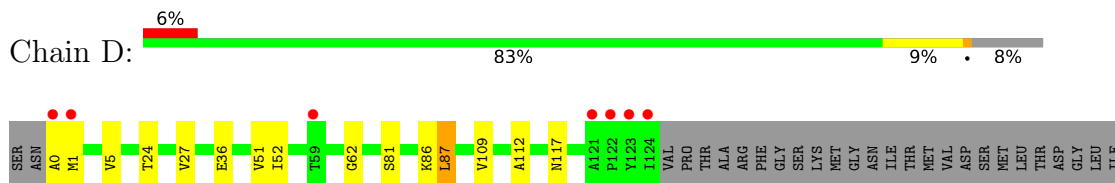
- Molecule 1: Acetoacetyl-CoA thiolase 2

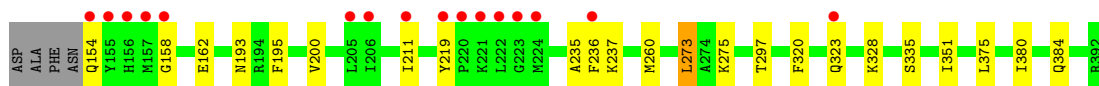


- Molecule 1: Acetoacetyl-CoA thiolase 2



- Molecule 1: Acetoacetyl-CoA thiolase 2





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.32Å 78.92Å 127.03Å 90.00° 112.73° 90.00°	Depositor
Resolution (Å)	39.05 – 2.00 39.05 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.05-2.00) 92.6 (39.05-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, $R_{free}$	0.175 , 0.207 0.173 , 0.204	Depositor DCC
$R_{free}$ test set	6283 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtrriage
Anisotropy	0.588	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	0/2916	0.83	5/3931 (0.1%)
1	B	0.55	0/2863	0.84	3/3860 (0.1%)
1	C	0.52	0/2696	0.83	8/3637 (0.2%)
1	D	0.44	0/2704	0.81	6/3646 (0.2%)
All	All	0.50	0/11179	0.83	22/15074 (0.1%)

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	ILE	N-CA-C	7.97	119.39	107.51
1	C	351	ILE	N-CA-C	7.24	117.37	110.42
1	B	87	LEU	CB-CA-C	-7.14	108.33	116.54
1	B	1	MET	N-CA-C	6.80	118.69	111.28
1	A	351	ILE	N-CA-C	6.72	116.87	110.42

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2878	0	2981	24	0
1	B	2831	0	2928	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2668	0	2762	23	0
1	D	2678	0	2767	30	0
2	A	17	0	0	6	0
2	B	15	0	0	0	0
2	C	15	0	0	5	0
2	D	17	0	0	7	0
3	A	245	0	0	2	0
3	B	259	0	0	2	0
3	C	243	0	0	1	0
3	D	127	0	0	1	0
All	All	11993	0	11438	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 85 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:GLU:HG2	1:D:237:LYS:HD2	1.61	0.81
1:A:-1:ASN:ND2	1:C:1:MET:HE3	2.06	0.70
1:A:62:GLY:HA2	1:C:87:LEU:HD11	1.74	0.69
1:D:162:GLU:CG	1:D:237:LYS:HD2	2.24	0.67
1:B:62:GLY:HA2	1:D:87:LEU:HD11	1.74	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/395 (98%)	381 (98%)	6 (2%)	0	100	100
1	B	381/395 (96%)	373 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	358/395 (91%)	353 (99%)	4 (1%)	1 (0%)	36	35
1	D	360/395 (91%)	351 (98%)	9 (2%)	0	100	100
All	All	1486/1580 (94%)	1458 (98%)	27 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	0	ALA

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/313 (98%)	305 (99%)	3 (1%)	68	75
1	B	301/313 (96%)	299 (99%)	2 (1%)	76	82
1	C	285/313 (91%)	283 (99%)	2 (1%)	76	82
1	D	284/313 (91%)	282 (99%)	2 (1%)	76	82
All	All	1178/1252 (94%)	1169 (99%)	9 (1%)	73	80

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	211	ILE
1	D	273	LEU
1	B	153	ASN
1	B	375	LEU
1	C	375	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	ASN

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Mol	Chain	Res	Type
1	B	188	ASN
1	D	68	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 64 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	388/395 (98%)	-0.18	18 (4%) 37 36	21, 32, 66, 104	3 (0%)
1	B	384/395 (97%)	-0.20	19 (4%) 35 34	19, 31, 61, 96	1 (0%)
1	C	363/395 (91%)	-0.10	18 (4%) 34 33	21, 34, 59, 103	1 (0%)
1	D	364/395 (92%)	0.36	23 (6%) 26 24	31, 46, 77, 107	0
All	All	1499/1580 (94%)	-0.04	78 (5%) 33 31	19, 36, 69, 107	5 (0%)

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	ILE	6.3
1	A	144	LEU	6.1
1	B	145	THR	5.9
1	D	220	PRO	5.5
1	D	222	LEU	5.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IOD	A	413	1/1	0.68	0.24	111,111,111,111	1
2	IOD	D	413	1/1	0.79	0.14	120,120,120,120	1
2	IOD	D	412	1/1	0.83	0.17	118,118,118,118	1
2	IOD	B	406[A]	1/1	0.85	0.14	77,77,77,77	1
2	IOD	B	406[B]	1/1	0.85	0.14	68,68,68,68	1
2	IOD	A	411	1/1	0.86	0.17	94,94,94,94	1
2	IOD	B	414	1/1	0.86	0.16	107,107,107,107	1
2	IOD	C	410	1/1	0.87	0.15	82,82,82,82	1
2	IOD	D	414	1/1	0.87	0.15	106,106,106,106	1
2	IOD	C	413	1/1	0.89	0.16	94,94,94,94	1
2	IOD	C	406	1/1	0.91	0.12	69,69,69,69	1
2	IOD	B	411	1/1	0.91	0.12	74,74,74,74	1
2	IOD	A	414	1/1	0.91	0.14	110,110,110,110	1
2	IOD	D	409	1/1	0.94	0.09	58,58,58,58	0
2	IOD	B	407	1/1	0.94	0.15	76,76,76,76	1
2	IOD	A	409	1/1	0.95	0.08	60,60,60,60	1
2	IOD	D	401	1/1	0.95	0.07	60,60,60,60	1
2	IOD	D	404	1/1	0.95	0.06	40,40,40,40	1
2	IOD	D	405[A]	1/1	0.95	0.14	40,40,40,40	1
2	IOD	D	405[B]	1/1	0.95	0.14	58,58,58,58	1
2	IOD	D	405[C]	1/1	0.95	0.14	56,56,56,56	1
2	IOD	A	412	1/1	0.95	0.10	81,81,81,81	1
2	IOD	C	408	1/1	0.95	0.07	46,46,46,46	1
2	IOD	B	413	1/1	0.95	0.10	62,62,62,62	1
2	IOD	C	412	1/1	0.95	0.18	68,68,68,68	1
2	IOD	A	408[B]	1/1	0.96	0.14	44,44,44,44	1
2	IOD	A	408[C]	1/1	0.96	0.14	60,60,60,60	1
2	IOD	C	414	1/1	0.96	0.14	69,69,69,69	1
2	IOD	D	411	1/1	0.96	0.08	80,80,80,80	1
2	IOD	C	407	1/1	0.96	0.17	76,76,76,76	1
2	IOD	A	407	1/1	0.96	0.09	48,48,48,48	1
2	IOD	A	408[A]	1/1	0.96	0.14	29,29,29,29	1
2	IOD	D	408[A]	1/1	0.97	0.07	44,44,44,44	1
2	IOD	D	408[B]	1/1	0.97	0.07	101,101,101,101	1
2	IOD	D	402	1/1	0.97	0.06	54,54,54,54	1
2	IOD	D	410	1/1	0.97	0.08	46,46,46,46	1
2	IOD	A	405	1/1	0.97	0.05	48,48,48,48	1
2	IOD	A	401	1/1	0.97	0.05	39,39,39,39	1
2	IOD	B	412	1/1	0.97	0.10	53,53,53,53	1
2	IOD	C	411	1/1	0.97	0.07	60,60,60,60	1
2	IOD	A	406	1/1	0.98	0.06	50,50,50,50	1
2	IOD	D	406	1/1	0.98	0.05	55,55,55,55	1
2	IOD	D	407	1/1	0.98	0.07	54,54,54,54	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IOD	C	401	1/1	0.98	0.05	38,38,38,38	1
2	IOD	C	403	1/1	0.98	0.06	44,44,44,44	1
2	IOD	B	409	1/1	0.98	0.05	51,51,51,51	1
2	IOD	B	410	1/1	0.98	0.04	46,46,46,46	1
2	IOD	D	403	1/1	0.98	0.04	38,38,38,38	1
2	IOD	B	404	1/1	0.98	0.05	46,46,46,46	1
2	IOD	A	404	1/1	0.98	0.04	37,37,37,37	0
2	IOD	A	410	1/1	0.98	0.07	63,63,63,63	1
2	IOD	C	409	1/1	0.99	0.02	45,45,45,45	1
2	IOD	B	401	1/1	0.99	0.07	45,45,45,45	1
2	IOD	B	402	1/1	0.99	0.04	50,50,50,50	1
2	IOD	B	408	1/1	0.99	0.04	42,42,42,42	1
2	IOD	C	402	1/1	0.99	0.05	41,41,41,41	0
2	IOD	B	403	1/1	0.99	0.03	28,28,28,28	1
2	IOD	C	415	1/1	0.99	0.04	63,63,63,63	1
2	IOD	C	404	1/1	0.99	0.04	28,28,28,28	1
2	IOD	C	405	1/1	0.99	0.04	45,45,45,45	1
2	IOD	A	402[B]	1/1	0.99	0.05	83,83,83,83	1
2	IOD	B	405	1/1	0.99	0.03	32,32,32,32	0
2	IOD	A	402[A]	1/1	0.99	0.05	43,43,43,43	1
2	IOD	A	403	1/1	1.00	0.04	28,28,28,28	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.